

Explicit matrix representation for the Hamiltonian of the one dimensional spin 1/2 Ising model in mutually orthogonal external magnetic fields.*

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Abstract

We derive an explicit matrix representation for the Hamiltonian of the Ising model in mutually orthogonal external magnetic fields, using as basis the eigenstates of a system of non-interacting spin 1/2 particles in external magnetic fields. We subsequently apply our results to obtain an analytical expression for the ground state energy per spin, to the fourth order in the exchange integral, for the Ising model in perpendicular external fields.

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1 Introduction

Field-induced effects in low-dimensional quantum spin systems have been studied for a long time [1, 2]. Hamiltonian models incorporating external magnetic fields are gaining popularity among experimentalists as well as theoreticians (see references [3, 4, 5, 6]). A longitudinal field is often introduced mainly to facilitate the calculation of order parameter and

associated susceptibility as can be seen for example in references [7, 8, 9], and a transverse field to introduce quantum fluctuations [10, 11].

Our main objective in this paper is to give an explicit matrix representation for the Hamiltonian of a system of N spin-1/2 particles on a cyclic one dimensional lattice chain, interacting via nearest neighbour exchange, in the presence of transverse and longitudinal external magnetic fields.

The Hamiltonian, H , is

$$H = -h_x \sum_{i=1}^N S_i^x - h_y \sum_{i=1}^N S_i^y - h_z \sum_{i=1}^N S_i^z - J \sum_{i=1}^N S_i^z S_{i+1}^z, \quad (1)$$

where h_x and h_y are the uniform external transverse magnetic fields, h_z is the uniform longitudinal field, J is the nearest neighbour exchange interaction, S_i are the usual spin-1/2 operators and the fields h_x , h_y and h_z are measured in units where the splitting factor and Bohr magneton are equal to unity. Periodic boundary condition is assumed so that $S_{N+i}^z \equiv S_i^z$, and so on. The parameters h_x , h_y , h_z and J are all assumed to be non-negative.

It is convenient to write $H = H_F + H_I$, where

$$H_I = -J \sum_{i=1}^N S_i^z S_{i+1}^z$$

and

$$H_F = -h_x \sum_{i=1}^N S_i^x - h_y \sum_{i=1}^N S_i^y - h_z \sum_{i=1}^N S_i^z.$$

H_F describes a system of N non-interacting spin 1/2 particles in mutually orthogonal external magnetic fields.

The model (1) has been widely studied for various combinations of the parameters h_x , h_y , h_z and J , especially for phase transitions (see [3, 5, 12] and the references therein). Our aim is to give an explicit matrix representation for H , using the eigenstates of H_F as basis.

Throughout this paper we will make use of the following identities which hold for $j, k \in \{0, 1\}$:

$$j \equiv \sin^2(j\pi/2), \quad 1 - j \equiv \cos^2(j\pi/2),$$

$$\delta_{jk} \equiv 1 - j - k + 2jk \equiv \cos^2\{(j - k)\pi/2\},$$

$$j + k - 2jk \equiv \sin^2\{(j - k)\pi/2\},$$

$$(-1)^j \delta_{jk} \equiv 1 - j - k \equiv \delta_{jk} - 2jk \equiv \cos\{(j + k)\pi/2\}, \quad (2)$$

$$\text{in particular } (-1)^j \equiv 1 - 2j \equiv \cos j\pi, \quad (-1)^{j-1} \equiv 2j - 1,$$

$$(-1)^j + (-1)^k \equiv 2(-1)^j \delta_{jk}, \quad (-1)^{j+k} \equiv 2\delta_{jk} - 1 \equiv \cos\{(j - k)\pi\},$$

$$j\delta_{jk} \equiv jk.$$

2 Quantization of a system of non-interacting spin 1/2 particles in external magnetic fields

A system of N non-interacting spin 1/2 particles in mutually orthogonal external magnetic fields h_x , h_y and h_z is described by the Kronecker sum Hamiltonian

$$H_F = H_{F_1} \oplus H_{F_2} \oplus \cdots \oplus H_{F_N}$$

where, for $j, k \in \{0, 1\}$, each single particle Hamiltonian H_{F_i} , at the i th site, has the matrix elements, in unit of \hbar ,

$$\begin{aligned} \langle \lambda_j | H_{F_i} | \lambda_k \rangle &= -\frac{h_z}{2} \cos j\pi \cos^2 \left\{ (j - k) \frac{\pi}{2} \right\} \\ &\quad - \left[\frac{a}{2} \cos^2 \left(\frac{j\pi}{2} \right) + \frac{a^*}{2} \cos^2 \left(\frac{k\pi}{2} \right) \right] \sin^2 \left\{ (j - k) \frac{\pi}{2} \right\} \end{aligned}$$

with respect to the eigenstates $\{|\lambda_0\rangle, |\lambda_1\rangle\}$ of the spin 1/2 operator S_i^z ,

whose elements, in unit of \hbar , are

$$\langle \lambda_j | S_i^z | \lambda_k \rangle = \frac{\cos j\pi}{2} \cos^2 \left\{ (j-k) \frac{\pi}{2} \right\} = \lambda_j \cos^2 \left\{ (j-k) \frac{\pi}{2} \right\} .$$

The remaining two spin 1/2 operators S_i^x and S_i^y have matrix elements given by

$$\begin{aligned} \langle \lambda_j | S_i^x | \lambda_k \rangle &= \frac{1}{2} \sin^2 \left\{ (j-k) \frac{\pi}{2} \right\} \\ \text{and} \\ \langle \lambda_j | S_i^y | \lambda_k \rangle &= \frac{-i \cos j\pi}{2} \sin^2 \left\{ (j-k) \frac{\pi}{2} \right\} . \end{aligned}$$

Parameters h_x , h_y and h_z are the external magnetic fields and $a = h_x - ih_y$.

Explicitly,

$$\begin{aligned} H_{F_i} &= -h_x S_i^x - h_y S_i^y - h_z S_i^z \\ &= -\frac{1}{2} \begin{pmatrix} h_z & h_x - ih_y \\ h_x + ih_y & -h_z \end{pmatrix} . \end{aligned}$$

2.1 Change of basis via the eigenstates of the single particle Hamiltonian

Solving the eigenvalue equation $H_{F_i} |\varepsilon_j\rangle = \varepsilon_j |\varepsilon_j\rangle$, the normalized eigenstates $|\varepsilon_j\rangle$, $j \in \{0, 1\}$, are found to be

$$|\varepsilon_j\rangle = ac_j |\lambda_0\rangle + b_j c_j |\lambda_1\rangle ,$$

with corresponding eigenvalues

$$\varepsilon_j = -h/2 \cos j\pi , \tag{3}$$

where

$$h = (h_x^2 + h_y^2 + h_z^2)^{1/2},$$

$$a = h_x - ih_y, \quad b_j = -h \cos j\pi - h_z$$

and

(4)

$$c_j = -\frac{\cos j\pi}{(2h)^{1/2} (h + h_z \cos j\pi)^{1/2}} = \frac{(h + h_z \cos j\pi)^{1/2}}{(2h)^{1/2} b_j}.$$

Note that

$$a^* a = -b_0 b_1 = h_x^2 + h_y^2 = h^2 - h_z^2,$$

$$a^* + a = 2h_x, \quad a^* - a = 2ih_y,$$

$$b_j b_k = (h + h_z \cos j\pi)^2 \cos^2 \left\{ (j - k) \frac{\pi}{2} \right\} - (h^2 - h_z^2) \sin^2 \left\{ (j - k) \frac{\pi}{2} \right\}$$

$$c_j c_k = \frac{1}{2h} \left(\frac{\cos^2 \{(j - k) \pi/2\}}{h + h_z \cos j\pi} - \frac{\sin^2 \{(j - k) \pi/2\}}{(h^2 - h_z^2)^{1/2}} \right),$$

and

$$a^* a \sum_{j=0}^1 c_j^2 = 1, \quad \sum_{j=0}^1 c_j^2 b_j = 0.$$

The diagonalizing matrix P has elements $P_{jk} = ac_k \cos^2(j\pi/2) + jb_k c_k$, for $j, k \in \{0, 1\}$. Thus, H_{F_i} is similar to the diagonal matrix D having elements $D_{jk} = \varepsilon_j \cos^2((j - k)\pi/2)$, that is

$$H_{F_i} = P D P^\dagger,$$

$$P = \begin{pmatrix} c_0 a & c_1 a \\ c_0 b_0 & c_1 b_1 \end{pmatrix}, \quad D = \begin{pmatrix} \varepsilon_0 & 0 \\ 0 & \varepsilon_1 \end{pmatrix}.$$

With respect to the new basis, $\{|\varepsilon_0\rangle, |\varepsilon_1\rangle\}$, and for $j, k \in \{0, 1\}$, the Pauli spin matrices have the representation

$$\begin{aligned}\langle \varepsilon_j | S_i^x | \varepsilon_k \rangle &= -\frac{h_x}{2h} \cos j\pi \cos^2 \left\{ (j-k) \frac{\pi}{2} \right\} \\ &\quad + [(h \cos j\pi + h_z) a + (h \cos k\pi + h_z) a^*] \frac{\sin^2 \{(j-k) \pi/2\}}{4h (h^2 - h_z^2)^{1/2}}, \\ \langle \varepsilon_j | S_i^y | \varepsilon_k \rangle &= -\frac{h_y}{2h} \cos j\pi \cos^2 \left\{ (j-k) \frac{\pi}{2} \right\} \\ &\quad + [(h \cos j\pi + h_z) a - (h \cos k\pi + h_z) a^*] \frac{i \sin^2 \{(j-k) \pi/2\}}{4h (h^2 - h_z^2)^{1/2}}\end{aligned}$$

and

$$\begin{aligned}\langle \varepsilon_j | S_i^z | \varepsilon_k \rangle &= -\frac{h_z}{2h} \cos j\pi \cos^2 \left\{ (j-k) \frac{\pi}{2} \right\} \\ &\quad - \frac{(h^2 - h_z^2)^{1/2}}{2h} \sin^2 \left\{ (j-k) \frac{\pi}{2} \right\}.\end{aligned}$$

2.2 General basis states for the matrix representation of one dimensional spin 1/2 Hamiltonian systems

Since H_F is a Hermitian operator that lives in a 2^N dimensional Hilbert space, \mathcal{H} , its eigenstates form a complete orthonormal basis, suitable for giving matrix representations for operators living in \mathcal{H} and with the same conditions at the boundary. The eigenvalue equation for H_F is

$$H_F |E_r\rangle = E_r |E_r\rangle, \quad r = 0, 1, 2, \dots, 2^N - 1.$$

For each r the eigenstate $|E_r\rangle$ is a direct product of the eigenstates of H_{F_i}

while the eigenvalue is the sum of the respective eigenvalues ε_i , that is

$$|E_r\rangle = |\varepsilon_{r_1}\rangle \otimes |\varepsilon_{r_2}\rangle \otimes \cdots \otimes |\varepsilon_{r_N}\rangle = \prod_{i=1}^N |\varepsilon_{r_i}\rangle$$

and

$$E_r = \varepsilon_{r_1} + \varepsilon_{r_2} + \cdots + \varepsilon_{r_N} = \sum_{i=1}^N \varepsilon_{r_i},$$

where

$$r_i = \sin^2 \left\{ \left(\left\lfloor \frac{r}{2^{N-i}} \right\rfloor \right) \frac{\pi}{2} \right\}, \quad i = 1, 2, \dots, N,$$

where $\lfloor z \rfloor$, the *floor* of z , is the smallest integer not greater than z . Thus each state $|E_r\rangle$ is uniquely represented by a binary vector $\mathbf{r} = (r_1, r_2, \dots, r_N)$.

Thus, any operator A in \mathcal{H} has the matrix representation A with elements given by

$$A_{rs} = \langle E_r | A | E_s \rangle.$$

Using (3) we get

$$E_r = h \sum_{i=1}^N r_i - \frac{Nh}{2} = hm_r - \frac{Nh}{2}. \quad (5)$$

Note that $m_r = \sum_{i=1}^N r_i$ counts the number of $|\varepsilon_1\rangle$ states in the direct product state $|E_r\rangle$. The degeneracy of the state $|E_r\rangle$ is therefore $g(E_r) = {}^N C_{m_r}$. Thus only the ground state and the most excited state are non-degenerate.

3 Quantization of the one dimensional spin 1/2 Ising model in external magnetic fields

Explicit matrix representation

Since H_F is diagonal in the basis $\{|E_r\rangle\}$, the only task is to find the matrix elements of H_I and then add them to those of H_F . We have

$$\begin{aligned} H_{I_{rs}} &= \langle E_r | H_I | E_s \rangle = -J \sum_{i=1}^N \langle E_r | S_i^z S_{i+1}^z | E_s \rangle \\ &= -J \sum_{i=1}^N d_{i_{rs}} S_{i_{r_i s_i}}^z S_{i+1_{r_{i+1} s_{i+1}}}^z, \end{aligned} \quad (6)$$

where $S_{k_{r_k s_k}}^z = \langle \varepsilon_{r_k} | S_k^z | \varepsilon_{s_k} \rangle$ and where we have introduced an N -dimensional vector \mathbf{d} whose components are $2^N \times 2^N$ symmetric binary matrices d_i defined by

$$d_{i_{rs}} = \prod_{\substack{j=1 \\ j \neq i \\ j \neq i+1}}^N \delta_{r_i s_i}. \quad (7)$$

Thus $d_{i_{rs}} = 1$ if either the two vectors \mathbf{r} and \mathbf{s} are one and the same vector, that is $\mathbf{r} = \mathbf{s}$, or they differ only at the consecutive i^{th} and $(i+1)^{th}$ entries, otherwise $d_{i_{rs}} = 0$.

Note that

$$\delta_{r_i s_i} \delta_{r_{i+1} s_{i+1}} d_{i_{rs}} = \delta_{r_i s_i} c_{i_{rs}} = \delta_{rs}, \quad (8)$$

where we have introduced another N -dimensional vector \mathbf{c} whose components are $2^N \times 2^N$ symmetric binary matrices c_i with elements given by

$$c_{i_{rs}} = \prod_{\substack{j=1 \\ j \neq i}}^N \delta_{r_i s_i}. \quad (9)$$

Thus $c_{i_{rs}} = 1$ if either the two vectors \mathbf{r} and \mathbf{s} are one and the same vector, $\mathbf{r} = \mathbf{s}$, or they differ only at the i^{th} component, otherwise $c_{i_{rs}} = 0$.

Motivated by the definitions in (7), (8) and (9) we introduce two more N -dimensional vectors, α and β , whose components are $2^N \times 2^N$ symmetric binary matrices, in terms of which the c_i and d_i matrices may also be expressed. The α_i and β_i matrices are defined through their elements by

$$\alpha_{i_{rs}} = \delta_{r_i s_i} = \cos^2 \{ (r_i - s_i) \pi / 2 \},$$

$$\beta_{i_{rs}} = \delta_{r_i s_i} \delta_{r_{i+1} s_{i+1}}$$

$$= \alpha_{i_{rs}} \alpha_{i+1_{rs}} = \cos^2 \{ (r_i - s_i) \pi / 2 \} \cos^2 \{ (r_{i+1} - s_{i+1}) \pi / 2 \}.$$

It is straightforward to verify the following properties for the α_i and β_i matrices:

$$\alpha_i \alpha_j = \alpha_j \alpha_i = 2^{N-1} \delta_{ij} \alpha_i + 2^{N-2} (1 - \delta_{ij}) J_{2^N},$$

$$\beta_i \beta_j = \beta_j \beta_i = 2^{N-2} \delta_{ij} \beta_i + (1 - \delta_{ij}) \{ 2^{N-3} \alpha_j \delta_{j,i+1} + (1 - \delta_{j,i+1}) 2^{N-4} J_{2^N} \}$$

and

$$\alpha_i \beta_j = \beta_j \alpha_i = 2^{N-2} \delta_{ij} \alpha_i + (1 - \delta_{ij}) \{ 2^{N-2} \alpha_i \delta_{i,j+1} + (1 - \delta_{i,j+1}) 2^{N-3} J_{2^N} \}, \quad (10)$$

where

$$J_{2^N} = \begin{pmatrix} 1 & 1 & \vdots & 1 \\ 1 & 1 & \vdots & 1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & \vdots & 1 \end{pmatrix}$$

is the $2^N \times 2^N$ *all-ones* matrix. The α_i and β_i matrices are singular and have trace equal to 2^N . The eigenvalues of α_i are 2^{N-1} repeated twice and 0 repeated $2^N - 2$ times while those of β_i are 2^{N-2} repeated four times and 0 repeated $2^N - 4$ times. Finally using multinomial expansion theorem and (10), it is readily established that the matrices $\alpha = \sum_{i=1}^N \alpha_i$

and $\beta = \sum_{i=1}^N \beta_i$ satisfy

$$\alpha^2 = 2^{N-1}\alpha + 2^{N-2}N(N-1)J_{2^N},$$

$$\beta^2 = 2^{N-2}(\alpha + \beta) + 2^{N-4}N(N-3)J_{2^N}$$

and

$$\alpha\beta = 2^{N-1}\alpha + 2^{N-3}N(N-2)J_{2^N}.$$

It is now obvious that

$$\begin{aligned} c_{i_{rs}} &= \delta_{rs} + (1 - \alpha_{i_{rs}}) \delta_{\alpha_{rs}, N-1} \\ &= \delta_{rs} + (1 - \alpha_{i_{rs}}) \delta_{\beta_{rs}, N-2} \\ &= \delta_{rs} + \delta_{\beta_{rs}, N-2} \cos^2(\alpha_{i_{rs}} \pi/2), \end{aligned} \tag{11}$$

$$\begin{aligned} d_{i_{rs}} &= \delta_{rs} + (1 - \alpha_{i_{rs}}) \alpha_{i+1_{rs}} \delta_{\beta_{rs}, N-2} \\ &\quad + (1 - \alpha_{i+1_{rs}}) \alpha_{i_{rs}} \delta_{\beta_{rs}, N-2} \\ &\quad + (1 - \alpha_{i_{rs}}) (1 - \alpha_{i+1_{rs}}) \delta_{\beta_{rs}, N-3} \end{aligned} \tag{12}$$

$$\begin{aligned} &= \delta_{rs} + \delta_{\beta_{rs}, N-3} + (\delta_{\beta_{rs}, N-2} - \delta_{\beta_{rs}, N-3})(\alpha_{i_{rs}} + \alpha_{i+1_{rs}}) \\ &\quad + (\delta_{\beta_{rs}, N-3} - 2\delta_{\beta_{rs}, N-2}) \alpha_{i_{rs}} \alpha_{i+1_{rs}}. \end{aligned}$$

From (11) and (12) we find

$$c_{rs} = \sum_{i=1}^N c_{i_{rs}} = N\delta_{rs} + \delta_{\beta_{rs}, N-2}$$

and

$$d_{rs} = \sum_{i=1}^N d_{i_{rs}} = N\delta_{rs} + 2\delta_{\beta_{rs}, N-2} + \delta_{\beta_{rs}, N-3}.$$

Explicitly

$$c_{i_{rs}} = \begin{cases} \cos^2(\alpha_{i_{rs}}\pi/2) & \text{if } \beta_{rs} = N - 2 \\ 0 & \text{if } \beta_{rs} < N - 2 \\ 1 & \text{if } r = s, \end{cases}$$

$$d_{i_{rs}} = \begin{cases} \cos^2(\alpha_{i_{rs}}\pi/2) \cos^2(\alpha_{i+1_{rs}}\pi/2) & \text{if } \beta_{rs} = N - 3 \\ \sin^2\{(\alpha_{i_{rs}} - \alpha_{i+1_{rs}})\pi/2\} & \text{if } \beta_{rs} = N - 2 \\ 0 & \text{if } \beta_{rs} < N - 2 \\ 1 & r = s, \end{cases}$$

$$c_{rs} = \begin{cases} 0 & \text{if } \beta_{rs} < N - 2 \\ 1 & \text{if } \beta_{rs} = N - 2 \\ N & \text{if } r = s \end{cases}$$

and

$$d_{rs} = \begin{cases} 0 & \text{if } \beta_{rs} < N - 3 \\ 1 & \text{if } \beta_{rs} = N - 3 \\ 2 & \text{if } \beta_{rs} = N - 2 \\ N & \text{if } r = s \end{cases}.$$

From the definitions of the c_i and d_i matrices the following additional properties are evident:

1. $c_i^n = 2^{n-1}c_i$, $d_i^n = 4^{n-1}d_i$, for $n \in \mathbb{Z}^+$.

2. The eigenvalues of c_i are 0 and 2, each repeated 2^{N-1} times while those of d_i are 0, repeated $2^N - 2^{N-2}$ times, and 4, repeated 2^{N-2} times.
3. The c_i and d_i matrices are singular and have trace 2^N .

Returning to (6) and substituting for the matrix elements $S_{k_{r_k} s_k}^z$, we find, after some algebra,

$$H_{I_{rs}} = -\frac{NJh_z^2}{4h^2}\delta_{rs} + \frac{Jh_z^2}{2h^2}\delta_{rs} \sum_{i=1}^N \sin^2 \{(r_i - r_{i+1})\pi/2\} \\ - (1 - \delta_{rs}) \frac{h_z J (h^2 - h_z^2)^{1/2}}{2h^2} P_{rs} + (1 - \delta_{rs}) \frac{J (h^2 - h_z^2)}{4h^2} Q_{rs},$$

where, (for $r \neq s$),

$$P_{rs} = \sum_{i=1}^N c_{i_{rs}} \cos \left\{ (r_{i-1} + r_{i+1}) \frac{\pi}{2} \right\} \\ = \delta_{\beta_{rs}, N-2} \cos \left\{ (r_{k-1} + r_{k+1}) \frac{\pi}{2} \right\}$$

and

$$Q_{rs} = \sum_{i=1}^N (2c_{i_{rs}} - d_{i_{rs}}) = 2c_{rs} - d_{rs} = -\delta_{\beta_{rs}, N-3},$$

where

$$k = \sum_{j=1}^N j (r_j - s_j)^2 = \sum_{j=1}^N j (1 - \delta_{r_j s_j}) = \sum_{j=1}^N j \sin^2 \left\{ (r_j - s_j) \frac{\pi}{2} \right\}.$$

Explicitly,

$$P_{rs} = \begin{cases} 1 & \text{if } \beta_{rs} = N - 2 \text{ and } r_{k-1} = 0 = r_{k+1} \\ 0 & \text{if } \beta_{rs} < N - 2 \text{ or } r_{k-1} + r_{k+1} = 1 \\ -1 & \text{if } r_{k-1} = 1 = r_{k+1} \end{cases}$$

and

$$Q_{rs} = \begin{cases} -1 & \text{if } \beta_{rs} = N - 3 \\ 0 & \text{if } \beta_{rs} < N - 3 \end{cases}.$$

Putting the results together we finally have the matrix elements for the Ising interaction Hamiltonian, H_I , to be explicitly given by

$$\begin{aligned} H_{I_{rs}} = & -\frac{NJ}{4} \frac{h_z^2}{h^2} \delta_{rs} + \frac{Jh_z^2}{2h^2} \delta_{rs} \sum_{i=1}^N \sin^2 \left\{ (r_i - r_{i+1}) \frac{\pi}{2} \right\} \\ & - (1 - \delta_{rs}) \frac{Jh_z (h^2 - h_z^2)^{1/2}}{2h^2} \delta_{\beta_{rs}, N-2} \cos \left\{ (r_{k-1} + r_{k+1}) \frac{\pi}{2} \right\} \\ & - (1 - \delta_{rs}) \frac{J(h^2 - h_z^2)}{4h^2} \delta_{\beta_{rs}, N-3}, \end{aligned}$$

where

$$k = \sum_{j=1}^N j \sin^2 \left\{ (r_j - s_j) \frac{\pi}{2} \right\}.$$

Since $H_{rs} = H_{F_{rs}} + H_{I_{rs}}$ we therefore have that the matrix elements of the Ising model in mutually orthogonal external magnetic fields are given by

$$\begin{aligned} H_{rs} = & h\delta_{rs} \sum_{i=1}^N r_i - \frac{Nh}{2} \delta_{rs} - \frac{NJ}{4} \frac{h_z^2}{h^2} \delta_{rs} + \frac{Jh_z^2}{2h^2} \delta_{rs} \sum_{i=1}^N \sin^2 \left\{ (r_i - r_{i+1}) \frac{\pi}{2} \right\} \\ & - (1 - \delta_{rs}) \frac{Jh_z (h^2 - h_z^2)^{1/2}}{2h^2} \delta_{\beta_{rs}, N-2} \cos \left\{ (r_{k-1} + r_{k+1}) \frac{\pi}{2} \right\} \\ & - (1 - \delta_{rs}) \frac{J(h^2 - h_z^2)}{4h^2} \delta_{\beta_{rs}, N-3}, \end{aligned}$$

with k as defined above.

Defining

$$f = \frac{h_z}{h}, \quad g = \frac{(h^2 - h_z^2)^{1/2}}{h}, \quad f^2 + g^2 = 1,$$

we have

$$\begin{aligned}
H_{I_{rs}} = & -\frac{NJf^2}{4}\delta_{rs} + \frac{Jf^2}{2}\delta_{rs} \sum_{i=1}^N \sin^2 \left\{ (r_i - r_{i+1}) \frac{\pi}{2} \right\} \\
& - (1 - \delta_{rs})\delta_{\beta_{rs}, N-2} \frac{Jfg}{2} \cos \left\{ (r_{k-1} + r_{k+1}) \frac{\pi}{2} \right\} \\
& - (1 - \delta_{rs}) \frac{Jg^2}{4} \delta_{\beta_{rs}, N-3}
\end{aligned} \tag{13}$$

and

$$\begin{aligned}
H_{rs} = & m_r h \delta_{rs} - \frac{Nh}{2} \delta_{rs} - \frac{NJf^2}{4} \delta_{rs} \\
& + \frac{Jf^2}{2} \delta_{rs} \sum_{i=1}^N \sin^2 \left\{ (r_i - r_{i+1}) \frac{\pi}{2} \right\} \\
& - (1 - \delta_{rs})\delta_{\beta_{rs}, N-2} \frac{Jfg}{2} \cos \left\{ (r_{k-1} + r_{k+1}) \frac{\pi}{2} \right\} \\
& - (1 - \delta_{rs}) \frac{Jg^2}{4} \delta_{\beta_{rs}, N-3} ,
\end{aligned} \tag{14}$$

where

$$m_r = \sum_{j=1}^N r_j, \quad k = \sum_{j=1}^N j \sin^2 \left\{ (r_j - s_j) \frac{\pi}{2} \right\}.$$

4 Example application: ground state energy of weakly interacting spin 1/2 particles in external magnetic fields

When the exchange integral J is small, the Ising interaction term H_I can be treated as a perturbation of H_F . In this section, we employ (13) to find

corrections, up to the fourth order in J , to the energy of the ground state of weakly interacting spin 1/2 particles in mutually orthogonal external magnetic fields. Since the ground state of H_F , the unperturbed system, is non-degenerate, we will apply the non-degenerate Rayleigh-Schrödinger perturbation theory.

The following particular cases of (13) will often be useful.

$$H_{I_{ss}} = -\frac{NJf^2}{4} + \frac{Jf^2}{2} \sum_{i=1}^N \sin^2 \left\{ (s_i - s_{i+1}) \frac{\pi}{2} \right\}. \quad (15)$$

In particular,

$$H_{I_{00}} = -\frac{Nf^2}{4} J. \quad (16)$$

For $s \neq t$

$$H_{I_{st}} = -\frac{fgJ}{2} \delta_{\beta_{st}, N-2} \cos \left\{ (s_{k-1} + s_{k+1}) \frac{\pi}{2} \right\} - \frac{g^2 J}{4} \delta_{\beta_{st}, N-3}, \quad (17)$$

where

$$k = \sum_{j=1}^N j \sin^2 \left\{ (r_j - s_j) \frac{\pi}{2} \right\}.$$

In particular,

$$H_{I_{0t}} = -\frac{fgJ}{2} \delta_{\beta_{0t}, N-2} - \frac{g^2 J}{4} \delta_{\beta_{0t}, N-3}. \quad (18)$$

Note also from (5) that

$$E_r - E_s = E_{rs} = (m_r - m_s)h, \quad E_{0s} = -m_s h. \quad (19)$$

4.1 First order correction to the energy

The first order correction to the energy of the ground state of H_F is the expectation value of the perturbation H_I in the ground state $|E_0\rangle$ of H_F .

Thus, quoting (16), we have

$$E_0^{(1)} = \langle H_I \rangle_{|E_0\rangle} = \langle E_0 | H_I | E_0 \rangle = H_{I_{00}} = -\frac{Nf^2}{4} J. \quad (20)$$

4.2 Second order correction to the energy

The second order correction to the energy of the ground state of H_F is given by

$$\begin{aligned} E_0^{(2)} &= \sum_{s=1}^{2^N-1} \frac{\langle E_0 | H_I | E_s \rangle \langle E_s | H_I | E_0 \rangle}{E_0 - E_s} \\ &= \sum_{s=1}^{2^N-1} \frac{|H_{I_{0s}}|^2}{E_{0s}}. \end{aligned}$$

According to (18),

$$H_{I_{0s}} = -\frac{fgJ}{2}\delta_{\beta_{0s}, N-2} - \frac{g^2J}{4}\delta_{\beta_{0s}, N-3}.$$

We therefore see that contributions to $E_0^{(2)}$ come only from states with either $m_s = \sum s_i = 1$ (corresponding to $\beta_{0s} = N - 2$) or $m_s = \sum s_i = 2$ (corresponding to $\beta_{0s} = N - 3$ in the case when the two $|\varepsilon_1\rangle$ states of the direct product state $|E_s\rangle$ are consecutive). A typical state with $m_s = 1$ is the state

$$|E_{2^{N-1}}\rangle = |\varepsilon_1\rangle |\varepsilon_0\rangle |\varepsilon_0\rangle \cdots |\varepsilon_0\rangle \cdots |\varepsilon_0\rangle \equiv (1, 0, 0, \dots, 0, \dots, 0)$$

while a particular state with $m_s = 2$ (and $\beta_{0s} = N - 3$) is the state

$$|E_{3 \times 2^{N-2}}\rangle = |\varepsilon_1\rangle |\varepsilon_1\rangle |\varepsilon_0\rangle \cdots |\varepsilon_0\rangle \cdots |\varepsilon_0\rangle \equiv (1, 1, 0, \dots, 0, \dots, 0).$$

Therefore

$$H_{I_{0, 2^{N-1}}} = -\frac{fgJ}{2} \text{ and } H_{I_{0, 3 \times 2^{N-2}}} = -\frac{g^2J}{4},$$

and since there are N vectors with $\beta_{0s} = N - 2$ and N vectors with $\beta_{0s} = N - 3$, and using (19), we obtain

$$\begin{aligned} E_0^{(2)} &= -\frac{N |H_{I_{0, 2^{N-1}}}|^2}{h} - \frac{N |H_{I_{0, 3 \times 2^{N-2}}}|^2}{2h} \\ &= -\frac{N f^2 g^2}{4h} J^2 - \frac{N g^4}{32h} J^2. \end{aligned} \tag{21}$$

The results (20) and (21) were also obtained in [13].

4.3 Third order correction to the energy

The third order correction to the energy of the ground state of H_F is obtainable from the formula

$$\begin{aligned}
E_0^{(3)} &= \sum_{s=1}^{2^N-1} \sum_{t=1}^{2^N-1} \frac{H_{I_{0s}} H_{I_{st}} H_{I_{t0}}}{E_{0s} E_{0t}} - H_{I_{00}} \sum_{s=1}^{2^N-1} \frac{|H_{I_{0s}}|^2}{E_{0s}^2} \\
&= \sum_{s=1}^{2^N-1} \frac{|H_{I_{0s}}|^2 H_{I_{ss}}}{E_{0s}^2} + 2 \sum_{s=1}^{2^N-2} \sum_{t=s+1}^{2^N-1} \frac{H_{I_{0s}} H_{I_{st}} H_{I_{t0}}}{E_{0s} E_{0t}} - H_{I_{00}} \sum_{s=1}^{2^N-1} \frac{|H_{I_{0s}}|^2}{E_{0s}^2} \\
&= S_1 + S_2 + S_3,
\end{aligned}$$

where

$$\begin{aligned}
S_1 &= \sum_{s=1}^{2^N-1} \frac{|H_{I_{0s}}|^2 H_{I_{ss}}}{E_{0s}^2}, \quad S_2 = 2 \sum_{s=1}^{2^N-2} \sum_{t=s+1}^{2^N-1} \frac{H_{I_{0s}} H_{I_{st}} H_{I_{t0}}}{E_{0s} E_{0t}}, \\
S_3 &= -H_{I_{00}} \sum_{s=1}^{2^N-1} \frac{|H_{I_{0s}}|^2}{E_{0s}^2}.
\end{aligned}$$

Note that in the above derivation we made use of the following summation identity

$$\sum_{s=a}^M \sum_{t=a}^M f_{st} = \sum_{s=a}^M f_{ss} + \sum_{s=a}^{M-1} \sum_{t=s+1}^M (f_{st} + f_{ts}).$$

Evaluation of S_1

- Contribution from states with $m_s = 1$ ($\Rightarrow \beta_{0s} = N - 2$)

$$H_{I_{0s}} = -\frac{fgJ}{2} \text{ (from (18))}, \quad H_{I_{ss}} = -\frac{Nf^2J}{4} + f^2J \text{ (from (15))}$$

The contribution of the N states with $m_s = 1$ to the sum S_1 is therefore

$$N \frac{f^2 g^2 J^2}{4} \left(-\frac{Nf^2J}{4} + f^2J \right) / h^2.$$

- Contribution from states with $m_s = 2$ (provided that $\beta_{0s} = N - 3$)

$$H_{I_{0s}} = -\frac{g^2 J}{4}, \quad H_{I_{ss}} = -\frac{N f^2 J}{4} + f^2 J$$

The N states with $m_s = 2$, $\beta_{0s} = N - 3$ therefore contribute

$$N \frac{g^4 J^2}{16} \left(-\frac{N f^2 J}{4} + f^2 J \right) / (4h^2)$$

to S_1 .

Putting these results together we have

$$\begin{aligned} S_1 = & \frac{N f^2 g^2 J^2}{4} \left(-\frac{N f^2 J}{4} + f^2 J \right) / h^2 \\ & + \frac{N g^4 J^2}{16} \left(-\frac{N f^2 J}{4} + f^2 J \right) / (4h^2). \end{aligned} \tag{22}$$

Evaluation of S_2

$$S_2 = 2 \sum_{s=1}^{2^N-2} \sum_{t=s+1}^{2^N-1} \frac{H_{I_{0s}} H_{I_{st}} H_{I_{t0}}}{E_{0s} E_{0t}}.$$

In each term of the sum, one of four different scenarios is possible, namely, $m_s = 1 = m_t$ or $m_s = 2 = m_t$ or $m_s = 1, m_t = 2$ or $m_s = 2, m_t = 1$. We look at each possible situation in turn.

- Contribution to S_2 when $m_s = 1 = m_t$

In this case, for each s vector, there are two possible t vectors for which the matrix element $H_{I_{st}}$ does not vanish, as typified below:

$$\left. \begin{array}{ll} s : (0, 1, 0, 0, \dots, 0, 0) & s : (0, 1, 0, 0, \dots, 0, 0) \\ t : (1, 0, 0, 0, \dots, 0, 0) & t : (0, 0, 1, 0, \dots, 0, 0) \end{array} \right\} \beta_{st} = N - 3.$$

In such a situation,

$$H_{I_{st}} = -\frac{g^2 J}{4}.$$

We also have

$$H_{I_{0s}} = -\frac{fgJ}{2}(s \neq 0, \beta_{0s} = N - 2)$$

and

$$H_{I_{t0}} = H_{I_{0t}} = -\frac{fgJ}{2}(t \neq 0, \beta_{0t} = N - 2).$$

Since there are N $m_s = 1$ states, the contribution to the sum S_2 when $m_s = 1 = m_t$ is

$$\begin{aligned} & (2N \cdot 2 \cdot -fgJ/2 \cdot -g^2J/4 \cdot -fgJ/2) / (-h \cdot -2h) \\ &= -\frac{Nf^2g^4J^3}{8h^2} \end{aligned}$$

- Contribution to S_2 when $m_s = 2 = m_t$

As in the previous case, for each s vector, there are only two possible t vectors for which the matrix element $H_{I_{st}}$ does not vanish, as typified below:

$$\left. \begin{array}{ll} s : (1, 1, 0, 0, \dots, 0, 0) & s : (1, 1, 0, 0, \dots, 0, 0) \\ t : (1, 0, 1, 0, \dots, 0, 0) & t : (0, 1, 0, 0, \dots, 0, 1) \end{array} \right\} \beta_{st} = N - 3.$$

In such a situation,

$$H_{I_{st}} = -\frac{g^2J}{4} \quad \text{but } H_{I_{t0}} = H_{I_{0t}} = 0 \text{ since } \beta_{t0} = N - 4.$$

There is therefore zero contribution to S_2 when $m_s = 2 = m_t$.

- Contribution to S_2 when $m_s = 2, m_t = 1$

In this case, typical situations with an s vector and the two t vectors for which $H_{I_{rs}}$ does not vanish are depicted below

$$\left. \begin{array}{ll} s : (1, 1, 0, 0, \dots, 0, 0) & s : (1, 1, 0, 0, \dots, 0, 0) \\ t : (0, 1, 0, 0, \dots, 0, 0) & t : (1, 0, 0, 0, \dots, 0, 0) \end{array} \right\} \beta_{st} = N - 2.$$

From (17) we have

$$H_{I_{st}} = -\frac{fgJ}{2} \cos(\pi/2) = 0,$$

signifying a zero contribution to the S_2 sum.

- Contribution to S_2 when $m_s = 1$, $m_t = 0$

Here as in the previous case we have $H_{I_{st}} = -fgJ/2 \cos(\pi/2) = 0$, so that again there is zero contribution to the S_2 sum.

Adding all the contributions we have

$$S_2 = -\frac{Nf^2g^4J^3}{8h^2}. \quad (23)$$

Evaluation of S_3

$$S_3 = -H_{I_{00}} \sum_{s=1}^{2^N-1} \frac{|H_{I_{0s}}|^2}{E_{0s}^2}$$

From (16), (18) and (19) we have immediately that

$$S_3 = \frac{Nf^2J}{4} \left(\frac{Nf^2g^2J^2}{4} \Big/ h^2 + \frac{Ng^4J^2}{16} \Big/ (4h^2) \right). \quad (24)$$

Finally combining (22), (23) and (24), we obtain the third order correction to the energy of the ground state of H_F as

$$E_0^{(3)} = -\frac{7Nf^2g^4J^3}{64h^2} + \frac{Nf^4g^2J^3}{4h^2}. \quad (25)$$

4.4 Fourth order correction to the energy

The fourth order correction to the energy of the ground state of H_F is given by the standard Rayleigh-Schrödinger perturbation formula

$$\begin{aligned} E_0^{(4)} = & \sum_{s=1}^{2^N-1} \sum_{t=1}^{2^N-1} \sum_{u=1}^{2^N-1} \frac{H_{I_{0s}}H_{I_{st}}H_{I_{tu}}H_{I_{u0}}}{E_{0s}E_{0t}E_{0u}} - H_{I_{00}} \sum_{s=1}^{2^N-1} \sum_{t=1}^{2^N-1} \frac{H_{I_{0s}}H_{I_{st}}H_{I_{t0}}}{E_{0s}E_{0t}^2} \\ & - H_{I_{00}} \sum_{s=1}^{2^N-1} \sum_{t=1}^{2^N-1} \frac{H_{I_{0s}}H_{I_{st}}H_{I_{t0}}}{E_{0s}^2E_{0t}} + H_{I_{00}}^2 \sum_{s=1}^{2^N-1} \frac{|H_{I_{0s}}|^2}{E_{0s}^3} - E_0^{(2)} \sum_{s=1}^{2^N-1} \frac{|H_{I_{0s}}|^2}{E_{0s}^2}. \end{aligned}$$

Calculations completely analogous to those in the previous sections, but much more involved, give $E_0^{(4)}$ as

$$E_0^{(4)} = -\frac{13Nf^2g^6}{192h^3}J^4 + \frac{55Nf^4g^4}{128h^3}J^4 - \frac{Nf^6g^2}{4h^3}J^4 - \frac{Ng^8}{2048h^3}J^4. \quad (26)$$

4.5 Approximate analytical expression for the ground state energy per spin for weakly interacting spin 1/2 particles in external magnetic fields

Adding the energy corrections (20), (21), (25) and (26) to the ground state energy (obtained by setting $m_r = 0$ in (5)) of the non-interacting spin 1/2 particles in external magnetic fields we therefore find, to the fourth order in the exchange integral, J , that the energy of the ground state, $E_{0_{IF}}$, of the one dimensional Ising model in mutually orthogonal external magnetic fields, for N spin sites is given by

$$E_{0_{IF}} \approx -\frac{Nh}{2} - \frac{Nf^2}{4}J - \frac{Nf^2g^2}{4h}J^2 - \frac{Ng^4}{32h}J^2 - \frac{7Nf^2g^4}{64h^2}J^3 + \frac{Nf^4g^2}{4h^2}J^3 \\ - \frac{13Nf^2g^6}{192h^3}J^4 + \frac{55Nf^4g^4}{128h^3}J^4 - \frac{Nf^6g^2}{4h^3}J^4 - \frac{Ng^8}{2048h^3}J^4,$$

that is

$$\frac{e_0}{\varepsilon_0} \approx 1 + \frac{f^2}{4}z + \left(\frac{g^2}{64} + \frac{f^2}{8}\right)g^2z^2 + \left(\frac{7f^2g^2}{256} - \frac{f^4}{16}\right)g^2z^3 \\ + \left(\frac{g^6}{16384} + \frac{13f^2g^4}{1536} - \frac{55f^4g^2}{1024} + \frac{f^6}{32}\right)g^2z^4,$$

where $e_0 = E_{0_{IF}}/N$ is the ground state energy per spin, $\varepsilon_0 = -h/2$ and $z = -J/\varepsilon_0$.

Since $f^2 + g^2 = 1$, we can also write

$$\frac{e_0}{\varepsilon_0} \approx 1 + \left(\frac{1}{4} - \frac{g^2}{4}\right)z + \left(\frac{1}{8} - \frac{7}{64}g^2\right)g^2z^2 \\ + \left(-\frac{1}{16} + \frac{39}{256}g^2 - \frac{23}{256}g^4\right)g^2z^3 \\ + \left(\frac{1}{32} - \frac{151}{1024}g^2 + \frac{161}{768}g^4 - \frac{4589}{49152}g^6\right)g^2z^4,$$

or, in a more compact form,

$$\frac{e_0}{\varepsilon_0} \approx 1 + \frac{f^2}{4}z + \sum_{m=2}^4 \left\{ z^m \sum_{k=0}^{m-1} (-1)^{m-k} c_k^{(m)} (g^2)^{k+1} \right\}, \quad (27)$$

with

$$c_0^{(m)} = \frac{(-1)^m}{2^{m+1}}, \quad m = 1, 2, \dots,$$

$$c_1^{(2)} = \frac{7}{64},$$

$$c_1^{(3)} = \frac{39}{256}, \quad c_2^{(3)} = \frac{23}{256}$$

$$c_1^{(4)} = \frac{151}{1024}, \quad c_2^{(4)} = \frac{161}{768}, \quad c_3^{(4)} = \frac{4589}{49152}.$$

Note that when $f = 0$, then

$$\frac{e_0}{\varepsilon_0} \approx 1 + \frac{1}{64}z^2 + \frac{1}{16384}z^4,$$

in perfect agreement with the exact result for the ground state energy of the transverse field Ising model [10]:

$$\frac{e_0}{\varepsilon_0} = \frac{(4+z)}{2\pi} \mathcal{E} \left[\frac{4\sqrt{z}}{4+z} \right] = 1 + \frac{1}{64}z^2 + \frac{1}{16384}z^4 + O(z^6),$$

where \mathcal{E} is a complete elliptic integral of the second kind.

The form of (27) suggests an exact result for the ground state energy per spin of the Ising model in external magnetic fields:

$$\frac{e_0}{\varepsilon_0} = 1 + \frac{f^2}{4}z + \sum_{m=2}^{\infty} \left\{ z^m \sum_{k=0}^{m-1} (-1)^{m-k} c_k^{(m)} (g^2)^{k+1} \right\},$$

where $c_k^{(m)}$ are positive rational numbers, and in particular, $c_0^{(m)} = (-1)^m / 2^{(m+1)}$ for $m \geq 2$.

4.6 Estimation of various order parameters for the Ising model in mutually orthogonal external magnetic fields

The knowledge of e_0 allows the derivation of approximate analytic expressions for physical quantities such as the magnetization in each direction and the spin-spin correlation function for neighbouring spins.

4.6.1 Magnetization

Invoking the Hellmann-Feynman rule in (1) gives for the x -magnetization

$$m_x = \frac{2}{N} \left\langle \sum_{i=1}^N S_i^x \right\rangle_{|E_{0_{IF}}\rangle} = -2 \frac{\partial e_0}{\partial h_x} = -2 \frac{\partial h}{\partial h_x} \frac{\partial e_0}{\partial h_x} = -2 \frac{h_x}{h} \frac{\partial e_0}{\partial h_x}$$

and similar expressions for m_y and m_z , the y - and z -magnetizations.

According to (27),

$$e_0 \approx -\frac{h}{2} - \frac{h}{8} z f^2 - \frac{h}{2} \sum_{m=2}^4 \left\{ z^m \sum_{k=0}^{m-1} (-1)^{m-k} c_k^{(m)} (g^2)^{k+1} \right\},$$

so that for $h \neq 0$ we obtain

$$\begin{aligned} \frac{\partial e_0}{\partial h} \approx & -\frac{1}{2} + \frac{z f^2}{4} \\ & + \sum_{m=2}^4 \left\{ z^m \sum_{k=0}^{m-1} (-1)^{m-k} c_k^{(m)} g^{2k} \left(-(k+1) f^2 + \frac{(m-1)}{2} g^2 \right) \right\}. \end{aligned} \quad (28)$$

Thus for $h_z < h \neq 0$,

$$m_z \approx f - \frac{z}{2} f^3 + \sum_{m=2}^4 \left\{ z^m \sum_{k=0}^{m-1} (-1)^{m-k} c_k^{(m)} g^{2k} (2(k+1) f^3 - (m-1) g^2 f) \right\},$$

and for $h_x < h \neq 0$ and $h_y < h \neq 0$, respectively,

$$m_x \approx \frac{h_x}{h} - \frac{z}{2} \frac{h_x}{h} f^2 + \frac{h_x}{h} \sum_{m=2}^4 \left\{ z^m \sum_{k=0}^{m-1} (-1)^{m-k} c_k^{(m)} g^{2k} (2(k+1) f^2 - (m-1) g^2) \right\}$$

and

$$m_y \approx \frac{h_x}{h} - \frac{z}{2} \frac{h_y}{h} f^2 + \frac{h_y}{h} \sum_{m=2}^4 \left\{ z^m \sum_{k=0}^{m-1} (-1)^{m-k} c_k^{(m)} g^{2k} (2(k+1)f^2 - (m-1)g^2) \right\}.$$

Note that in the absence of interaction, $(z = 0, h \neq 0)$, $m_x^2 + m_y^2 + m_z^2 = 1$.

4.6.2 Nearest neighbour spin-spin correlation

The spin-spin correlation, $c_{i,i+1}$, is given by

$$c_{i,i+1} = \frac{4}{N} \left\langle \sum_{i=1}^N S_i^z S_{i+1}^z \right\rangle_{|E_{0_{IF}}\rangle} = -4 \frac{\partial e_0}{\partial J} = -4 \frac{\partial z}{\partial J} \frac{\partial e_0}{\partial z} = -\frac{8}{h} \frac{\partial e_0}{\partial z},$$

yielding

$$c_{i,i+1} = f^2 + 4 \sum_{m=2}^4 \left\{ m z^{m-1} \sum_{k=0}^{m-1} (-1)^{m-k} c_k^{(m)} (g^2)^{k+1} \right\}.$$

Note that in the absence of interaction, $z = 0$, we have $c_{i,i+1} = f^2$ while $h = h_z$ gives $c_{i,i+1} = 1$.

5 Conclusion

We have given an explicit matrix representation for the Hamiltonian of the Ising model in mutually orthogonal external magnetic fields, with basis the eigenstates of a system of non-interacting spin 1/2 particles in external magnetic fields. We subsequently applied our results to obtain an analytical expression for the ground state energy per spin, to the fourth order in the exchange integral, for the Ising model in perpendicular external fields. Since the Hamiltonian of the non-interacting spin 1/2 particles in external magnetic fields is a Hermitian operator that lives in a 2^N dimensional Hilbert space, its eigenstates form a complete orthonormal basis, suitable for giving matrix representations for any operator living in the same Hilbert space and with the same conditions at the boundary.

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